On-going developments in Code_Saturne® for modelling oxycombustion processes

Sandro Dal Secco, Jorge Santamaría

Saturne User’s Club

Chatou, 1st December 2008
Outline

- Combustion and energy supply
- Fossil fuels and oxycombustion
- Requirements for oxyfiring vs. air firing
- Adapting Code_Saturne® to oxy-combustion
- First tests of the combustion model (axisymmetrical pulverised coal jet flame)
- Conclusions and future work
Combustion

- Combustion is a “complex sequence of exothermic chemical reactions between a fuel and an oxidant accompanied by the production of heat or both heat and light”.

- In the large majority of the real world uses of combustion, the oxygen (O₂) oxidant is obtained from the ambient air and the resultant flue gas from the combustion will contain nitrogen:

  **Methane combustion**: \( \text{CH}_4 + 2\text{O}_2 + 7.52\text{N}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 7.52\text{N}_2 + \text{heat} \)

- As can be seen, when air is the source of the oxygen, nitrogen is by far the largest part of the resultant flue gas.
In reality, combustion processes are never perfect or complete. In flue gases from combustion of carbon (as in coal combustion) or carbon compounds (as in combustion of hydrocarbons, wood etc.) both unburned carbon (as soot) and carbon compounds (CO and others) will be present. Also, when air is the oxidant, some nitrogen can be oxidized to various nitrogen oxides ($\text{NO}_x$). Sulphur and nitrogen are present in coal and can be oxidized to various oxides ($\text{NO}_x$, $\text{SO}_x$).

\[
\text{coal} + \text{air} \rightarrow \text{carbon dioxide} + \text{water vapour} + \text{NO}_x + \text{SO}_x + \text{soot} + \text{CO} + \text{ash}
\]
Energy supply

- Security of energy supply
- Availability (long and short term)
- Competitiveness

Not only costs but also related to its degree of supply security and environmental advantage

Regarding all stages (from production through transportation to utilization)
Combustion of fossil fuels

- security of energy supply
- competitiveness
- environmental acceptability

Emissions:

- particulates → respiratory health
- \( \text{NO}_x, \text{SO}_2 \) → acid rain
- \( \text{CO}_2 \) → greenhouse effect
CO$_2$ capture and storage (CCS)

- Precombustion
  - Air separation
  - Gasification

- Postcombustion
  - CO$_2$ capture from flue gases (CO$_2$ absorbents)

- Oxycombustion
  - Air separation
  - Combustion with pure oxygen
A clever environmental solution: Oxycombustion

- Almost no emission to the atmosphere
  (Particulates, NO\textsubscript{x}, SO\textsubscript{x}, CO\textsubscript{2})
- In the frame of CO$_2$ capture technologies EDF favours oxycombustion as the most promising option for coal power plants in the mid-term perspective.

- CFD simulations is an important tool for the optimisation and better design of a boiler. Code_Saturne® is EDF’s Open Source CFD solution for 3D fluid dynamics and combustion calculations.
Introduction

Requirements for oxyfiring vs. air firing

- Different flue gases atmosphere: **higher CO₂ and H₂O concentrations**
  - Radiative properties \( f(\text{CO}_2, \text{H}_2\text{O}) \)
  - Heat capacities: \( C_p^{\text{CO}_2}, C_p^{\text{H}_2\text{O}} > C_p^{\text{N}_2} \)
  - Chemical reactions:
    - Heterogeneous reactions:
      \[
      \text{C(s)} + \text{CO}_2 \rightarrow 2\text{CO} \\
      \text{C(s)} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2
      \]
    - Homogeneous reactions:
      \[
      \text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2 \quad \text{(Water-gas shift reaction)} \\
      \text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2
      \]
Introduction

Requirements for oxyfiring vs. air firing

- Devolatilization
  - Higher mass loss under CO\textsubscript{2} atmosphere rather than under N\textsubscript{2} atmosphere (DTF measurements)

- Char combustion
  - Heterogeneous reactions with CO\textsubscript{2} and water vapour:
    - \( C(s) + CO_2 \rightarrow 2CO \) ➤ Already implemented
    - \( C(s) + H_2O \rightarrow CO + H_2 \) ➤ Future developments

- Flue gas recirculation
  - Increase in water vapour content
  - Flue gas mass flow rate
Adapting Code_Saturne® to oxy-combustion

- Enhancement of the algorithm for the kinetics to equilibrium in $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ reaction

- Implementation of the heterogeneous oxidation of char by $\text{CO}_2$

- Possibility to deal with different oxidizers in the inlet conditions (air, oxygen, flue gases)

- Future developments:
  - Implementation of the heterogeneous reaction with water vapour
  - Evaluation of the assumptions between kinetic and diffusive limitations
Adapting Code_Saturne® to oxy-combustion

- **Combustion models:**

- **Gas phase reactions:**

  \[ \text{CH}_{X_1} + \text{O}_2 \rightarrow \text{CH}_{X_2} + \text{H}_2\text{O} \quad \text{(low temperature devolatilization)} \]

  \[ \text{CH}_{X_2} + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O} \quad \text{(high temperature devolatilization)} \]

  \[ \text{CO} + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{CO}_2 \]

- **Heterogeneous reactions:**

  \[ \text{C(s)} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO} \]

  \[ \text{C(s)} + \text{CO}_2 \rightarrow 2\text{CO} \]

**New features for oxy-combustion**
First tests of the combustion model in an axisymmetrical pulverised coal jet flame

- Simple geometry: a cylinder, which allows axisymmetrical treatment and therefore reduces to 2D case (15000 cells) for a 1,20 m long combustion chamber

- New reactions and kinetics in the combustion model have been tested for several configurations:
  - Air firing
  - Nitrogen replaced by CO₂ (same volumetric proportions as in air)
  - Nitrogen replaced by CO₂ (same mass proportions)
  - Oxy-combustion similar conditions (with recycled gases)
First tests of the combustion model in an axisymmetrical pulverised coal jet flame

- New features in the combustion model were tested one-by-one in order to quantify the importance of both reactions.

<table>
<thead>
<tr>
<th>Case</th>
<th>Reaction 1: CO + 1/2O₂ ⇌ CO₂</th>
<th>Reaction 2: C(s) + CO₂ → 2CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A</td>
<td>instantaneous kinetics</td>
<td>not used</td>
</tr>
<tr>
<td>Case B</td>
<td>global kinetics</td>
<td>not used</td>
</tr>
<tr>
<td>Case C</td>
<td>global kinetics</td>
<td>taken into account</td>
</tr>
</tbody>
</table>
First tests of the combustion model in an axisymmetrical pulverised coal jet flame

- Inlet conditions for the 4 types of flame:

<table>
<thead>
<tr>
<th></th>
<th>Air</th>
<th>CO2 [%w]</th>
<th>CO2 [%vol]</th>
<th>Oxy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary oxidant</td>
<td>Air</td>
<td>O$_2$+2,39 CO$_2$</td>
<td>O$_2$+3,76 CO$_2$</td>
<td>O$_2$+0,3N$_2$+0,7H$_2$O+2,4CO$_2$</td>
</tr>
<tr>
<td>Secondary oxidant</td>
<td>Air</td>
<td>O$_2$+2,39 CO$_2$</td>
<td>O$_2$+3,76 CO$_2$</td>
<td>O$_2$+0,2N$_2$+0,5H$_2$O+1,2CO$_2$</td>
</tr>
<tr>
<td>Primary mass flow [kg/s]</td>
<td>1,9E-3</td>
<td>1,9E-3</td>
<td>1,9E-3</td>
<td>1,9E-3</td>
</tr>
<tr>
<td>Secondary mass flow [kg/s]</td>
<td>9,3E-3</td>
<td>9,3E-3</td>
<td>1,05E-2</td>
<td>6,7E-3</td>
</tr>
<tr>
<td>Coal mass flow [kg/s]</td>
<td>9,0E-4</td>
<td>9,0E-4</td>
<td>9,0E-4</td>
<td>9,0E-4</td>
</tr>
</tbody>
</table>
Case A: Instantaneous kinetics for CO/CO₂ and without oxidation of char by CO₂

Temperature [K]

Partial pressure O₂

Oxy

CO₂ [%w]

Heterogeneous combustion rate

Air

CO₂ [%vol]

unburned carbon in ash

CO concentration [% mass]
Case B: Global kinetics for CO/CO$_2$ and without oxidation of char by CO$_2$
Case C: Global kinetics for CO/CO$_2$ and taking into account the oxidation of char by CO$_2$
Conclusions:

- First developments in the combustion model for Code_Saturne® have been successfully adapted in order to model oxy-combustion processes.

- Several flames have been used to test the different models one-by-one.

- A very different combustion behaviour has been observed when air is no more the diluting gas. CO₂ (vol.) leads to incomplete combustion because of the high dilution and decrease of temperature. Nevertheless combustion in CO₂ (mass) atmosphere is more efficient than air firing. Finally, under oxy-combustion conditions, the quantity of diluted gases being definitely lower, combustion is more effective than in the case of combustion in air.

- Taking into account or not the kinetics of CO oxidation seems to have more influence on the results than the heterogeneous reaction of CO₂ and char. However, the kinetics used here do not correspond to any real case of combustion of a specific coal. It will be advisable to get realistic values for this kinetics from experiments in Drop Tube Furnaces.
Future Work:

- Due to the high water vapour content in recycled flue gases in oxy-combustion processes, the heterogeneous gasification of char by water vapour should be studied:

  \[ C_{(s)} + H_2O \rightarrow H_2 + CO \]

- Regarding combustion regimes, due to the fact that all different reactants (\(O_2\), \(H_2O\) and \(CO_2\)) not have the same reactivity towards carbon in the char, the assumption of similar regime (bulk-surface diffusion, pore diffusion or reaction control) could be not correct.

- It is likely that high temperature gasification with \(H_2O\) or \(CO_2\) is kinetically controlled, or in the transition region, while the \(O_2\) reaction with carbon is in the diffusion-controlled regime at the same temperature.

- For the purpose of model validation we take part in projects involving oxifiring facilities (Oxycoal, IFRF)
Practical example:
Modelling the E.ON UK’s 1 MWth CTF with Code_Saturne®

- Calculations made in frame of the british project Oxycoal

- 500 000 cells
Velocity and temperature in middle plane (air firing)

Large internal recirculation zone
Velocity and temperature in middle plane (oxy firing)

Smaller external recirculation zones

Lower temperature and flame shifted